Stripe Formation in Electron-Doped Cuprates

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We investigate the formation of charge domain walls in an electron-doped extended Hubbard model for the superconducting cuprates. Within an unrestricted Hartree-Fock approach, extended by slave bosons to obtain a better treatment of strong correlations, we demonstrate the occurrence of stripes in the $(1, 1)$ and $(1, -1)$ directions having one doped electron per stripe site. The different filling, direction, and width of these electron-doped stripes with respect to those obtained in the hole-doped systems have interesting observable consequences.

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The issue of charge inhomogeneity in the cuprates and particularly in the underdoped region of their phase diagram is presently attracting great attention from both the experimental [1] and the theoretical [2–4] point of view.

On the experimental side, there is direct evidence for the occurrence of (static or dynamic) charge ordering in under- and optimally doped cuprates [1], from extended x-ray absorption fine structure [5], neutron scattering [6], x-ray scattering [7,8], nuclear quadrupolar resonance (NQR) [9], and magnetotransport [10,11]. This evidence is particularly compelling for hole-doped materials at the specific doping $1/8$, where commensurability effects between the charge ordering and the underlying lattice make the charge order particularly robust [12], and gives rise to (a partially) insulating character (this is the so-called $1/8$ phenomenon). This commensurability effect seems instead much less evident in the electron-doped materials.

The stripe instability was predicted theoretically in Ref. [13] within Hartree-Fock (HF) theory applied to the extended Hubbard model and confirmed by a number of subsequent investigations [14]. Only recently, however, the occurrence in the single-band Hubbard model of half-filled stripes (i.e., with half a hole per stripe site) in the (1,0) [or equivalently in the (0,1)] direction [half-filled-vertical stripes (HFVS)] was demonstrated within a generalized HF approach including slave bosons to suitably handle the strong local electron-electron interaction [15]. This result showed that (a proper treatment of) strong correlations and long-range interactions are crucial in determining a specific stripe texture similar to the one observed in the cuprates. Obviously it is desirable that the variational (and therefore uncontrolled) results obtained within the HF–slave-boson scheme will be supported by other numerical techniques (e.g., exact diagonalization or Monte Carlo). Nevertheless this approach is a valuable tool allowing for a systematic analysis of large clusters of not too schematic models.

The aim of the present work is to apply the same joint HF–slave-boson technique to investigate the stripe formation in a more realistic extended three-band Hubbard model in the case of electronic doping. It is to be borne in mind that in any HF approach the solutions are self-consistently stabilized by locating the chemical potential in the middle of a gap. Therefore this approach is only suitable to describe insulating phases where the filling and/or the breaking of translational symmetry gives rise to such gaps. In the present work we intend to describe by our method the $1/8$ commensurate systems where both the charge ordering and the (nearly) insulating character are substantial.

The model and the main outcomes.—The extended three-band Hubbard model in hole picture reads

$$H = \sum_{\langle ij\rangle\sigma} t_{ij}^{pd}(d_{i\sigma}^{\dagger} p_{j\sigma} + \text{H.c.}) + \sum_{\langle jj'\rangle\sigma} t_{jj'}^{pp}(p_{j\sigma}^{\dagger} p_{j'\sigma} + \text{H.c.}) + \Delta \sum_{j\sigma} p_{j\sigma}^{\dagger} p_{j\sigma} + U_d \sum_i d_{i\uparrow}^{\dagger} d_{i\uparrow} d_{i\downarrow}^{\dagger} d_{i\downarrow} + U_p \sum_j p_{j\uparrow}^{\dagger} p_{j\uparrow} p_{j\downarrow}^{\dagger} p_{j\downarrow} + \frac{1}{2} \sum_{i\neq j,\sigma\sigma'} V_{ij} c_{i\sigma}^{\dagger} c_{i\sigma} c_{j\sigma'}^{\dagger} c_{j\sigma'} . \quad (1)$$

The first and second terms describe the nearest neighbor (nn) copper-oxygen and oxygen-oxygen hopping of holes in the $3d_{x^2-y^2}$ copper orbitals and in the $2p_{x,y}$ oxygen orbitals, respectively. Δ is the energy difference between p and d orbitals (the energy of the d orbitals is set to zero), while U_d (U_p) is the local Hubbard repulsion between holes on the same copper (oxygen) orbital. The last term is the long-range interaction, with $V_{ij} = Ve^{-r_{ij}/\lambda_S}/(2r_{ij})$, with r_{ij} being the distance between two sites and λ_S is the screening length. V is set to $V = U_{pd}e^{1/\lambda_S}$ in order to match the U_{pd} nn Cu-O repulsion. In this term, the c operators represent d or p hole operators depending on the nature of the site.

In the cuprates the $3d^8$ configuration is the highest in energy due to the large repulsion between holes on the same copper site. Therefore, following the procedure of Ref. [15], we treat the strong local hole-hole repulsion U_d

by means of the slave-boson technique in the Kotliar-Ruckenstein formulation [16], where four auxiliary bosonic fields, e_i, $s_{i,\uparrow}$, $s_{i,\downarrow}$, and D_i, are introduced for each copper site i. These operators stand for the annihilation of empty, singly occupied states with spin up or down, and doubly occupied sites (in hole picture), respectively. Since there are only four possible states per copper site, these boson projection operators must satisfy the completeness constraints $e_i^\dagger e_i + \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} + D_i^\dagger D_i = 1$ and $n_{i\sigma} = s_{i\sigma}^\dagger s_{i\sigma} + D_i^\dagger D_i$ ($n_{i\sigma}$ is the hole-density operator on Cu sites). In the saddle point approximation the four auxiliary boson fields are treated as numbers. Because of the weaker strength of the repulsion and the smaller average hole density on oxygen sites, the other interaction terms, U_p and V, are treated by a standard HF decoupling. The effective one-particle Hamiltonian can be diagonalized by the transformation $c_{i,\sigma} = \sum_k \Phi_{i,\sigma}(k) a_k$ where the fermion wave functions $\Phi_{i,\sigma}(k)$ obey the orthonormality constraint $\sum_{i,\sigma} \Phi_{i\sigma}^*(k)\Phi_{i\sigma}(q) = \delta_{kq}$. The equivalent procedure adopted here is to minimize the total energy with respect to the fermionic wave functions and to the bosonic fields within the orthonormality and completeness constraints. The minimization is carried out in real space on finite clusters allowing for complete freedom of the local charge densities, of the local magnetizations, and of the local boson mean-field values [17].

We summarize here the main results valid both for hole and electron doping. (i) As in the single-band Hubbard model [15], also in the three-band Hubbard model the major effect of the slave-boson treatment is to stabilize the stripes with respect to isolated spin polarons. Indeed the Gutzwiller-like procedure implemented via the slave bosons allows the charge to delocalize without paying a much too large repulsive energy. Then, since general arguments [18] show that the charge mobility tends to favor stripes with respect to isolated spin polarons, stripes are not artificially disfavored within our approach. The same is not true in standard HF treatments, where the double occupancy of the sites is avoided via a strong antiferromagnetic (AF) polarization of the spins, which greatly suppresses the intersite hopping. (ii) For the same reason the static local magnetization is generically less pronounced in the present approach and, consistently with the experimentally observed stripes [6], the antiferromagnetically correlated spins are in antiphase in adjacent domains separated by a charge stripe. (iii) For moderate to large values of U_d, the natural energy scale for charge excitations no longer is U_d, but rather the charge-transfer energy Δ becomes the principal parameter determining the stability of stripes with respect to an ordered lattice (Wigner crystal) of maximally separated spin polarons. The stripes are stable only below a critical value Δ_c, depending on the other parameters of the model, which in any reasonable realistic case is much larger than the critical values obtained in the standard (i.e., without slave bosons) HF technique. The reason for the relevance of Δ is again related to the effect of the kinetic energy in stabilizing the stripes: When the charge-transfer energy Δ is too large the charge mobility is suppressed and the configuration with isolated polarons becomes more favorable. (iv) For a quite broad range of realistic values of the parameters the HFVS and the filled diagonal stripes (FDS) [i.e., with one hole per stripe site and running along the $(1, 1)$ or $(1, -1)$ directions] are the most stable or the only stable solutions. In particular, *for hole doping* $x = 1/8$, while the standard HF treatment favors the FDS, it is found that *the HFVS become the ground state when strong correlations are properly treated by slave bosons.* The absolute stability of HFVS occurs even in the absence of long-range interactions. In this respect, the hole-doped three-band Hubbard model seems more favorable than the single-band one in giving rise to half-filled stripes of the type observed in hole-doped cuprates. (v) The local repulsion on oxygen plays only a minor role, while (vi) the oxygen-oxygen hopping t_{pp} enhances the charge mobility and therefore stabilizes the stripes with respect to the polaron Wigner crystal (POLWC). Regarding the "long-range" interactions, it was found that a nn repulsion U_{pd} naturally disfavors the stripes while it does not affect the POLWC, where the charges are at a larger distance. Nevertheless (vii) a moderate U_{pd} destabilizes the HFVS less than the FVS, thus strengthening the stability of the HFVS. On the other hand, (viii) the large-distance part of a truly long-range interaction turns out to increase the energy of the POLWC, thus favoring further the stability of an array of stripes.

Finally, the effects of a coupling between holes and static lattice deformations were also investigated. In particular, the hopping was modulated by the displacement of oxygen ions in the j site along the Cu-O bonds $t_{ij}(\{u_j\}) = t_{pd} \pm \alpha u_j$, where the sign is positive if the Cu-O distance is decreased, while it is negative if the Cu-O distance increases. For simplicity, in this model we neglected the coupling between the O-O hopping and the lattice. In an analogous way the orbital energy on the copper site is modified as $\epsilon_i(\{u_k\}) = \epsilon_d + \beta \sum_j (\pm u_j)$. Then the dimensionless hole-lattice couplings are $\lambda_\alpha = \alpha^2/(Kt_{pd})$ and $\lambda_\beta = \beta^2/(Kt_{pd})$. At variance with the findings of Ref. [19], where stripe textures were found only as *local* minima, the slave-boson treatment produces *absolutely* stable stripe solutions. However, owing to the specific choice of lattice displacement, there occurs a frustration effect whenever holes (or electrons) are located on neighboring sites. This frustration of the lattice displacement is not present in the case of distant polarons. Therefore, (ix) the electron-phonon coupling lowers the energy of stripe configurations less than it lowers the POLWC, so that it is detrimental for stripes (particularly for the filled ones) in comparison to the POLWC. Nevertheless, the absolute stability of HFVS at hole doping $x = 1/8$ survives in the presence of a moderate coupling.

For concreteness, we report in Table I the energy difference between the HFVS or the FDS and the POLWC

TABLE I. Energy differences per doped hole between two different stripe configurations (HFVS and FDS) and the POLWC in a 8×8 (HFVS) or 9×8 (FDS) lattice with periodic boundary conditions. The parameter values are $t_{pd} = 1.3$ eV, $t_{pp} = 0.65$ eV, $\Delta = 3.6$ eV, $U_d = 10.5$ eV, $U_p = 4$ eV [Ref. [20], (HSC)]. The LR coupling is such that $U_{pd} = 1.2$ eV with a screening length $\lambda_S = 32$ lattice units. The EP couplings are $\lambda_\alpha = 0.5$ and $\lambda_\beta = 0$.

	$\epsilon_{\mathrm{HFVS}} - \epsilon_{\mathrm{POLWC}}$ (eV)	$\epsilon_{\mathrm{FDS}} - \epsilon_{\mathrm{POLWC}}$ (eV)
HSC	-0.036	$+0.003$
LR	-0.084	No minimum
EP	$+0.009$	$+0.034$
EP + LR	-0.034	No minimum

configurations at $x = 1/8$ for a typical set of parameters. The HFVS stabilization effect of the long-range (LR) interaction is shown in the second line, while the destabilization due to the electron-phonon (EP) coupling is shown in the third line. The consideration of all the different interactions leads to a stable HFVS configuration as indicated in the fourth line. As shown in the last column, the FDS are instead always disfavored with respect to the POLWC.

Electron doping.—While the above analysis was carried out mostly for hole doping (and particularly for $x = 1/8$), it is quite important to extend the investigation to electron-doped systems. While the general validity of the above results is maintained, some important specific features are also found. In particular, it was noticed that the charge in electron-doped stripes is more localized. A comparison of the charge profile of hole-doped (HD) and electron-doped (ED) stripes is shown in Fig. 1, where the narrower charge distribution of ED stripes is apparent. This effect

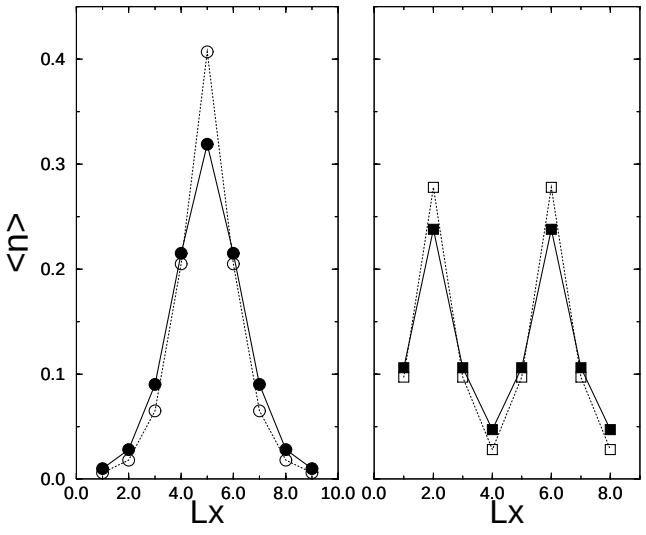

FIG. 1. Charge density profile in the $(1,0)$ direction for FDS (left panel) and for HFVS (right panel) for both ED (empty symbols) and HD (filled symbols) systems. The parameters are the same as in Table I with $x = \pm 1/8$, but with $\lambda_\alpha = \lambda_\beta = 0$.

is natural since the doped holes reside mostly on oxygen sites where due to the smaller interaction and to the direct t_{pp} hopping they acquire a high mobility, while the doped electrons reside mostly on copper sites. Therefore the doped-electron mobility is lower because it occurs only via an intermediate charge transfer to oxygen sites. One main consequence is that the stripe formation is generically more difficult. Nevertheless, stripe textures still remain the ground state for realistic values of the parameters. In particular, even in the presence of a sizable electron-lattice coupling (which, as discussed above, favors the POLWC solution more than the stripes) stable FDS textures are found. A second important effect is that *FDS (with one doped electron per stripe site) become more stable than the HFVS.* This latter finding suggests that ED cuprates should be more similar to the nickelates, where diagonal stripes with one doped hole per site are detected.

Discussion.—The fact that FDS accommodate one doped charge per site, rather than one-half like the HFVS, increases the (average) distance between the stripes. For instance, at $|x| = 1/8$, in the FDS case the stripes are at distance $d_{\mathrm{FDS}} = 8a/\sqrt{2}$, while the HFVS are separated by $d_{\mathrm{HFVS}} = 4a$. As a consequence the antiferromagnetic background between stripes is better preserved when FDS are formed. This effect is emphasized by the stronger confinement of the charge inside the ED stripes.

The formation of ordered arrays of stripes is naturally accompanied by a spin response, which appears in neutron scattering at momenta displaced by an amount ε from the AF wave vector $Q_{\mathrm{AF}} = (\pm\pi/a, \pm\pi/a)$. While this effect has indeed been observed in metallic HD materials, with $\varepsilon \sim x$ for x up to $1/8$ and then saturating ($\varepsilon \sim$ const), comparatively detailed neutron scattering data are not available for ED systems. Our findings suggest that the incommensurate spin-excitation peaks should be closer in k space, with the incommensurate momenta scaling as $\varepsilon \sim x/\sqrt{2}$. Moreover, while in HD materials the peaks appear in the $(1,0)$ and $(0,1)$ directions consistently with the vertical ordering of the stripes, in ED materials the corresponding peaks should be observed in the $(1,1)$ and $(1,-1)$ directions, according to our finding of diagonal stripe formation. However, the substantial disorder effects due to pinning could broaden the spin peaks making the observation of incommensurability more difficult. In this respect more local probes like the NQR (successfully applied in the HD materials [9]) can be more powerful tools for detecting charge inhomegeneities.

Although no theory is presently available for the scattering due to (dynamically fluctuating) stripes, if the results obtained here for the insulating commensurate systems keep some validity in the metallic phase, some speculative remarks can be done on transport properties. The first generic observation is that the narrower charge distribution of stripes in ED systems indicates a smaller transversal mobility. This is because the stronger confinement of the electrons inside the ED stripe makes it more difficult

for the electrons to delocalize on neighbor sites driving the stripe meandering. This, together with the larger separation of the filled ED stripes could explain why the antiferromagnetic phase is quite more robust upon electron doping than upon hole doping stressing the analogy between the stripes in ED systems and in nickelates. As far as transport along the stripes is concerned, it can be noticed that HFVS should be more metallic than FDS. This is expected because in the longitudinal direction HFVS are similar to an array of quarter-filled one dimensional wires. If these wires escape the longitudinal charge-density wave commensurate instability, these 1D structures should naturally be more metallic than 1D chains with an empty or a full band [21].

The metallic properties of ED stripes should also be strongly affected by disorder effects, which are expected to be more relevant than in HD stripes since the ED stripes are less mobile and more anharmonic. In this regard, the recent observation [22] that small amounts of interstitial apical oxygen suppress superconductivity (but not metallicity) giving rise to pseudogap effects is of obvious relevance. A natural speculation could be that the interstitial oxygen triggers a pinning of the stripes. The suppression of stripe *fluctuations* then induces the suppression of superconductivity giving rise to a metallic (nonsuperconducting) state with disordered static (and locally well-formed) stripes with the consequent stronger reduction of density of states near the Fermi level.

Another generic consequence is that the diagonal stripes of the ED systems should display rather different commensurability effects than in the HD materials. This is a consequence of the different spacing and ordering direction as well as of the different T' crystal structure of the ED cuprates. In particular, in the ED case, the $1/8$ effects are not expected to be marked [23] since the stripes are quite far apart and the collective nature of the ordered state is likely affected by disorder pinning.

In conclusion, the occurrence of stripes in a rather realistic model for ED cuprates is a quite intriguing finding. According to our results, the specific features of the stripes in ED materials are different from the features of stripes in HD ones. Therefore, if the occurrence of stripes in electron-doped systems will be experimentally confirmed, the comparison with the stripes already observed in the hole-doped materials will likely shed light on the physical mechanisms acting in both ED and HD cuprates. This calls for a search of experimental signatures and characterization of stripes in ED cuprates.

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